How to make a protein structure file (.psf) and lammps data file (.dat) file for a CNT on graphene (or any graphene nanostructure)

First check out Axel Kohlmeyer's TOPO tutorial tools webpages:

General: http://sites.google.com/site/akohlmey/software/topotools

and

Tutorial: http://sites.google.com/site/akohlmey/software/topotools/topotools-tutorial---introduction

We'll be pulling heavily from Tutorials 1 and 2. It might be helpful to try to follow all the steps he outlines to help understand what we are going to do next.

How to make the .psf and .dat files.

1. output your structure from Nanoengineer2 as either an xyz or pdb file.
2. Open VMD from the directory containing the xyz or pdb file.
3. Type the following commands in the VMD command console

   package require topotools
   package require pbctools

4. Open your pdb or xyz file with the following command

   mol new yourfile.xyz.or.pdb autobonds yes waitfor ll

5. Next create all the atom selections. For nanotubes we have carbon and hydrogen bonded in benzene rings. CB and HA are the standard CHARMM atom types for this type of bonding. To select the atoms type the following series of commands:

   set selh [atomselect top {name H}]
   $selh set type HA
   $selh set mass 1.00800
   $selh set charge 0.0

   set selc [atomselect top {name C}]
   $selc set type CB
   $selc set mass 12.01100
   $selc set charge 0.0

   set sel [atomselect top all]

6. The next thing you need to do is manually add bonds to make the graphene sheet periodic. In other words you have to draw connections between the carbons on the left side of the graphene sheet to the corresponding atoms on the right side of the sheet. The same thing for atoms at the top and the bottom of the sheet. To do this go to the VMD Main window. Click “Mouse”, then click “Add/Remove Bonds” Then click pairs of atoms that your want to bond. If you

accidentally click the wrong atom, which is easy to do, click it again and it should delete the bond.

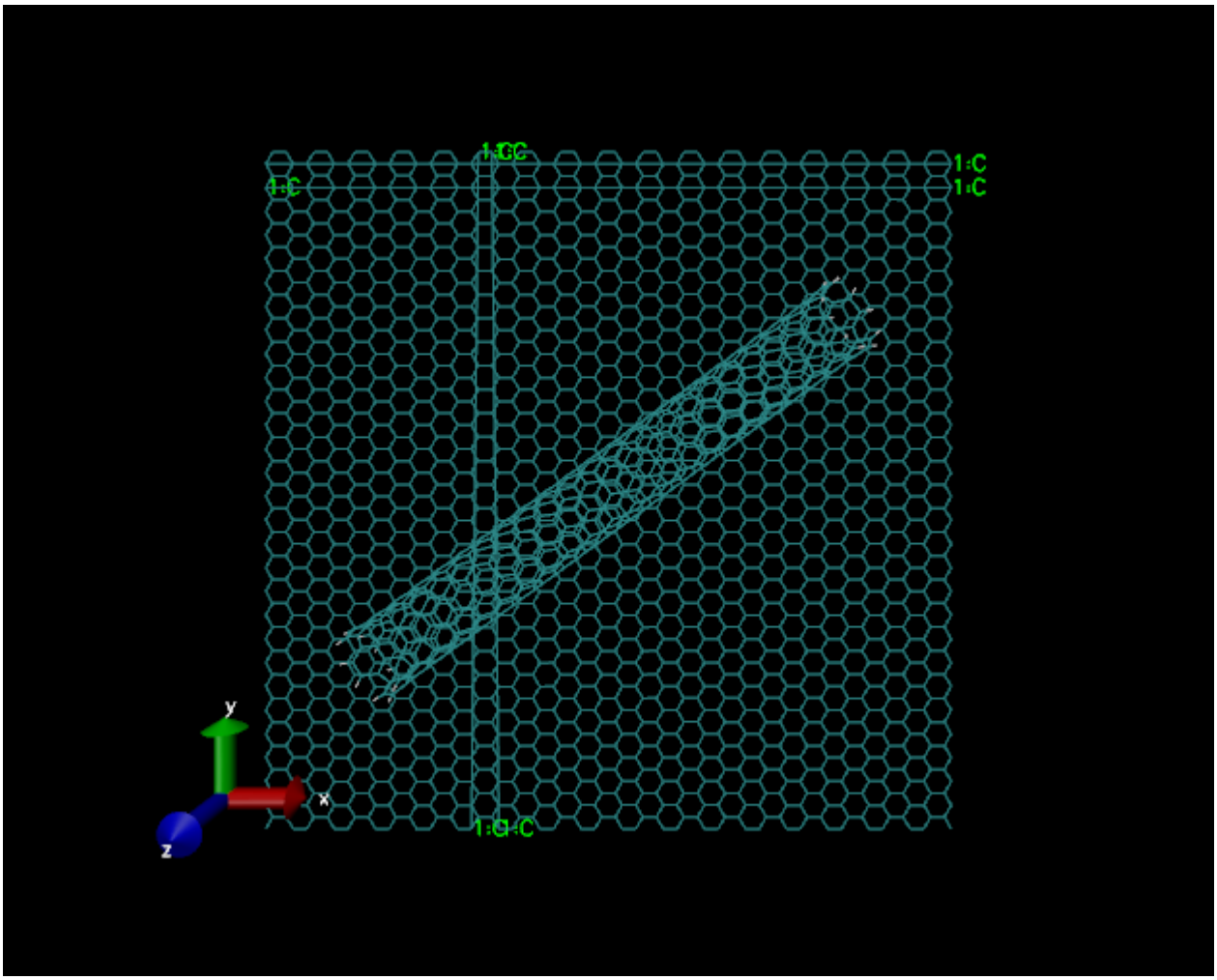
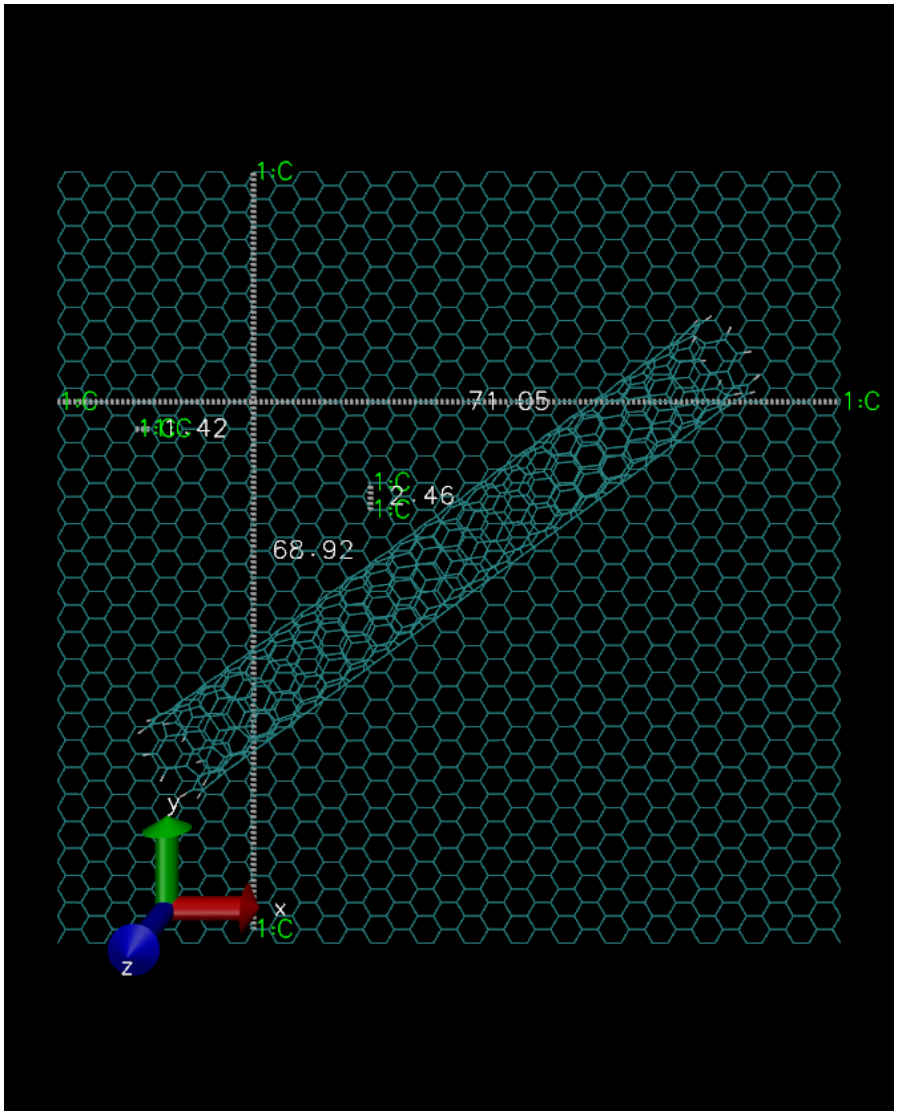


Fig 1. Draw bonds from left to right and top to bottom until all atoms right at the edge are connected.

7. Next get the periodic boundary dimensions. This is the length and height of the graphene sheet + 1 repeat unit. To measure the dimensions, go to VMD Main, click “Mouse”, “Label”, the select bonds. You need to measure and record 4 things.
    1. Far right to far left
    2. The length of a single bond (left to right)
    3. Top to bottom, making sure that pick the same atom column. You should have one extra carbon row, not included in the measurement.
    4. The height of one hexagon.
    (NOTE: if your graphite lattice is not oriented in the same way as the one in the figure below, swap top bottom with left right in the above instructions.

The periodic dimensions of your system are then x= 1+2 and y = 3+4. For lammps it asks for xhi, xlo, etc. It's standard to center the system, so divide x or y by 2, so that xhi = x/2 and xlo = -x/2, etc.



8. Next we need to set the bond types, angle types, and dihedral types. Topotools does this for us by calling the following commands:

   topo retype bond
   topo bondtypenames (see if the output makes sense. You should have CB-CB and CB-HA type bonds)
   topo guessangles
   topo guessdihedrals

That should be everything required to create the output files, so finally:

9. Output the dat and psf files by typing the following commands:

   topo writelammpsdat yournewfile.dat full
   animate write psf yournewfile.psf

10. The last thing you need to do is manually enter the period boundary lengths into the lammps

.dat file. Open the yournewfile.dat in an editor and replace the xlo, xhi, etc with the values you found in step 7. You ahould also set zhi and zlo to some reasonable value. You need enough height so you can move the haptic device. I think -5 and +30 should work fine.

That's it.